

SEARCH REQUEST FORM

8-400 ✓

Requestor's
Name:

Mark Clardy

Serial

Number: 08/537,843

Date:

8/26/96

Phone:

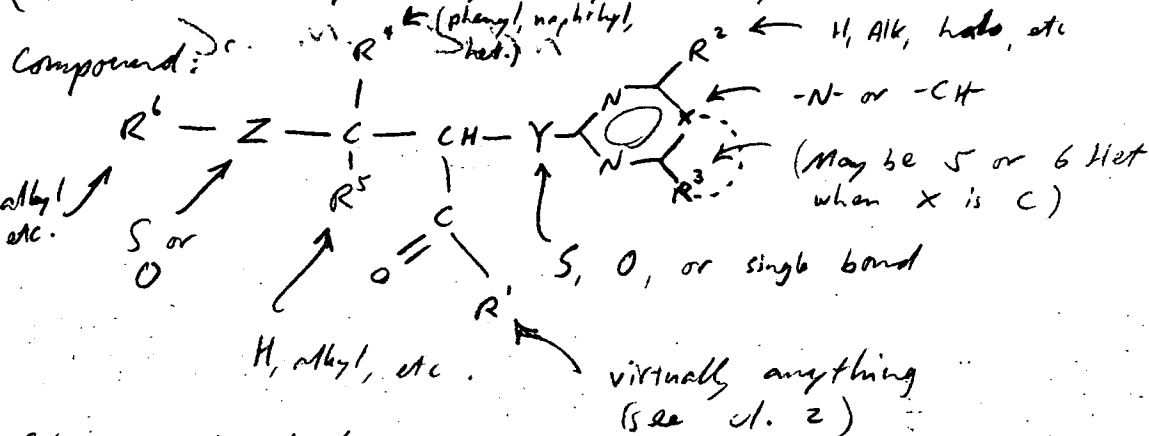
?

Art Unit:

Search Topic:

Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevant citations, authors keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevant claim(s).

(Herbicidal) Compound/Composition/Method.

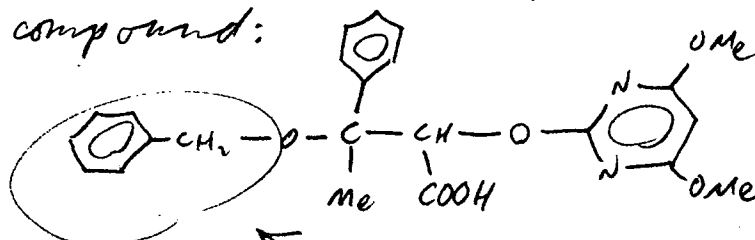


Claims attached

Face of file attached.

All refs are
P.D. (or later, in
same inv.)

Tested compound:

prior art
(EP-A 409 368)

has methyl instead of benzyl here

STAFF USE ONLY

19

Date completed:

APR 8

Searcher:

9-5-96

Terminal time:

Elapsed time:

CPU time:

Total time:

Number of Searches:

Number of Databases:

Search Site

STIC

CM-1

Pre-S

Type of Search

N.A. Sequence

A.A. Sequence

Structure

Bibliographic

Vendors

IG Suite

STN

Dialog

APS

Geninfo

SDC

DARC/Questel

Other

Clardy 08/537,843

=> del his

(FILE 'REGISTRY' ENTERED AT 07:29:37 ON 05 SEP 96)

DEL HIS Y
ACT CLARDY/A

L1 STR
L2 190 SEA FILE=REGISTRY SSS FUL L1

ACT CLARDY2/A

L3 STR
L4 (190) SEA FILE=REGISTRY SSS FUL L3
L5 STR
L6 17 SEA FILE=REGISTRY SUB=L4 SSS FUL L5

FILE 'HCAPLUS' ENTERED AT 07:41:52 ON 05 SEP 96

L7 11 S L2
L8 2 S L6
L9 9 S L7 NOT L8

=> fil reg

~~FILE 'REGISTRY'~~ ENTERED AT 07:42:15 ON 05 SEP 96
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 1996 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 02 SEPT 96 HIGHEST RN 180310-23-0
DICTIONARY FILE UPDATES: 04 SEPT 96 HIGHEST RN 180310-23-0

TSCA INFORMATION NOW CURRENT THROUGH DECEMBER 1995

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

=> d his 11-16

(FILE 'REGISTRY' ENTERED AT 07:29:37 ON 05 SEP 96)

DEL HIS Y
ACT CLARDY/A

L1 STR
L2 190 SEA FILE=REGISTRY SSS FUL L1

ACT CLARDY2/A

L3 STR
L4 (190) SEA FILE=REGISTRY SSS FUL L3
L5 STR

broad search

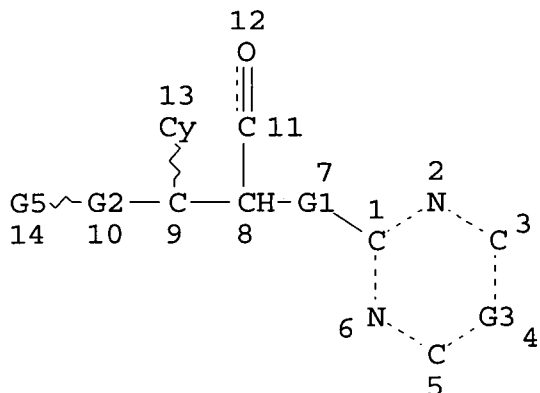
Clardy 08/537,843

L6 17 SEA FILE=REGISTRY SUB=L4 SSS FUL L5

tested compound

=> d que stat 12

L1 STR



REP G1=(0-1) Q

VAR G2=O/S

VAR G3=N/C

VAR G5=C/CB

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L2 190 SEA FILE=REGISTRY SSS FUL L1

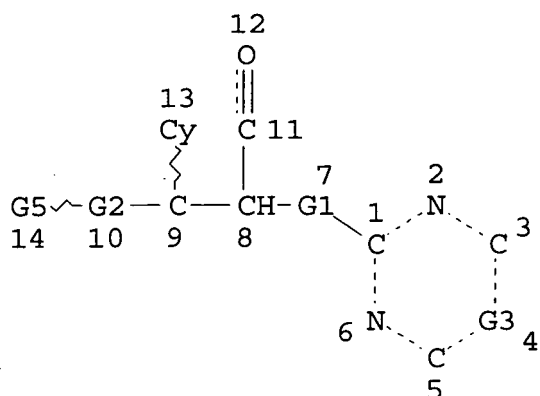
100.0% PROCESSED 62595 ITERATIONS

190 ANSWERS

SEARCH TIME: 00.01.06

=> d que stat 16

L3 STR



REP G1=(0-1) Q

VAR G2=O/S

VAR G3=N/C

VAR G5=C/CB

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

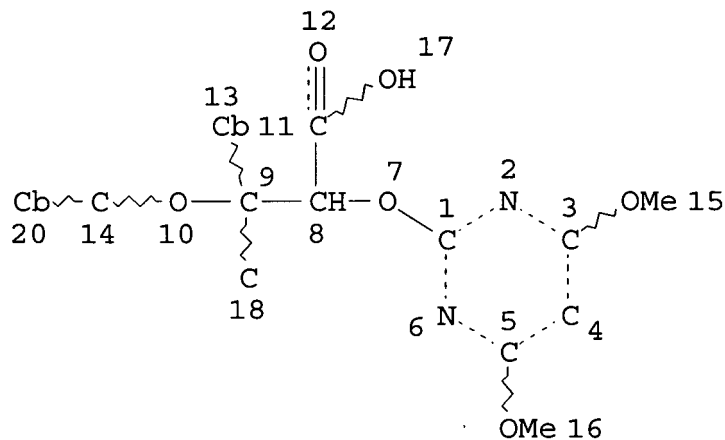
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L4 (190)SEA FILE=REGISTRY SSS FUL L3

L5 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 13

Clardy 08/537,843

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
L6 17 SEA FILE=REGISTRY SUB=L4 SSS FUL L5

100.0% PROCESSED 157 ITERATIONS
SEARCH TIME: 00.00.03

~~17~~ ANSWERS

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 07:42:27 ON 05 SEP 96
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 1996 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1967 - 5 Sep 1996 VOL 125 ISS 11
FILE LAST UPDATED: 5 Sep 1996 (960905/ED)

Meeting Abstracts for Orlando ACS Meeting Now in HCAPLUS. Please
see NEWS for details.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d hisl l7-
'HISL' IS NOT A VALID FORMAT FOR FILE 'HCAPLUS'
'L7-' IS NOT A VALID FORMAT FOR FILE 'HCAPLUS'
ENTER DISPLAY FORMAT (BIB):end

=> d his l7-

(FILE 'REGISTRY' ENTERED AT 07:29:37 ON 05 SEP 96)

FILE 'HCAPLUS' ENTERED AT 07:41:52 ON 05 SEP 96
L7 11 S L2
L8 2 S L6 narrower struct.
L9 9 S L7 NOT L8 broad struct

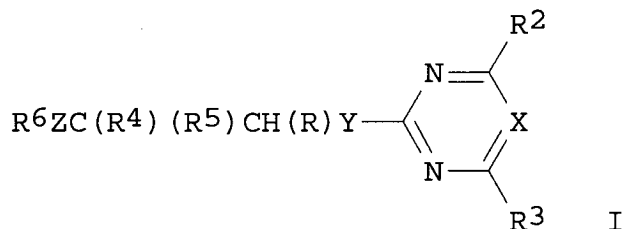
FILE 'REGISTRY' ENTERED AT 07:42:15 ON 05 SEP 96

FILE 'HCAPLUS' ENTERED AT 07:42:27 ON 05 SEP 96

=> d all l8 1-2

L8 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 1996 ACS
AN 1995:916669 HCAPLUS
DN 123:307319

TI Carboxylic acid derivatives as inhibitors of endothelin binding to receptors *Inv.*
 IN Baumann, Ernst; Vogelbacher, Uwe Josef; Rheinheimer, Joachm; Klinge, Dagmar; Riechers, Hartmut; Kroeger, Burkhard; Bialojan, Siegfried; Bollschweiler, Claus; Wernet, Wolfgang; et al.
 PA BASF A.-G., Germany
 SO Ger. Offen., 31 pp.
 CODEN: GWXXBX
 PI DE 4411225 A1 951005
 AI DE 94-4411225 940331
 DT Patent
 LA German
 IC ICM A61K031-505
 ICS A61K031-53
 CC 2-10 (Mammalian Hormones)
 Section cross-reference(s): 34
 OS MARPAT 123:307319
 GI



AB Carboxylic acid derivs. I [R = CHO, CO₂H, group hydrolyzable to CO₂H; R₂, R₃ = halo, C1-4 alkyl, C1-4 alkoxy, C1-4 haloalkoxy, C1-4 alkylthio; X = N, CR₁₄; R₄ = (substituted) C1-10 alkyl, (substituted) C3-12 cycloalkyl or cycloalkenyl, (substituted) C3-6 alkenyl or alkynyl, (substituted) heterocyclyl, (substituted) Ph or naphthyl; R₅ = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, or R₄ and R₅ complete a 3-8-membered ring; R₆ = (substituted) alkyl, (substituted) alkenyl, (substituted) alkynyl, (substituted) cycloalkyl; R₁₄ = H or forms an O-contg. 3-4-membered alkylene or alkenylene chain with R₃; Y = S, O, single bond; Z = S, O] are prep'd. as inhibitors of endothelin binding to receptors for treatment of e.g. (pulmonary) hypertension, acute myocardial infarct, Raynaud's syndrome, atherosclerosis, and asthma. Thus, I (R₁ = CO₂H, R₂ = R₃ = OMe, R₄ = Ph, R₅ = Me, R₆ = 4-isopropylphenyl, X = CH, Y = Z = O) inhibited binding of endothelin to endothelin A receptors of cloned human CHO cells and endothelin B receptors of guinea pig cerebellar membranes with K_i 2.5 .times. 10⁻⁷ and 3.0 .times. 10⁻⁶M, resp. I (R = CO₂Me, R₂ = R₃ = OMe, R₄ = R₆ = Ph, R₅ = H, X = CH, Y = S, Z = O) was prep'd. by reaction of Me

3-phenoxy-3-phenyl-2-hydroxybutyrate (prepn. given) with MeSO₂Cl and 4,6-dimethoxypyrimidine-2-thiol.

ST pyrimidinylalkanecarboxylate prepn endothelin receptor inhibitor

IT Antihypertensives

Vasodilators
(carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT Receptors
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(ETA (endothelin, A), carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT Blood vessel, disease
(Raynaud's phenomenon, carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT Bronchodilators
(antiasthmatics, carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT Antiarteriosclerotics
(antiatherosclerotics, carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT Antihypertensives
(pulmonary, carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT 123626-67-5, Endothelin 1
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT 170296-15-8P
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT 159308-02-8P 159308-03-9P 159308-04-0P 159308-05-1P
159308-06-2P 159308-07-3P 159308-08-4P 159308-09-5P
159308-10-8P 159308-11-9P 159308-12-0P 159308-13-1P
159308-14-2P 159308-15-3P 159308-16-4P 159308-17-5P
159308-18-6P 159308-19-7P 159559-14-5P 159559-15-6P
170296-16-9P 170296-17-0P 170296-18-1P 170296-19-2P
170296-20-5P 170296-21-6P 170296-22-7P 170296-23-8P
170296-24-9P 170296-25-0P 170296-26-1P 170296-27-2P
170296-28-3P 170296-29-4P 170296-30-7P 170296-31-8P
170296-32-9P 170296-33-0P 170296-34-1P 170296-35-2P
170296-36-3P 170296-37-4P 170296-38-5P 170296-39-6P
170296-40-9P 170296-41-0P **170296-42-1P** 170296-43-2P
170296-44-3P 170296-45-4P **170296-46-5P**
170296-47-6P **170296-48-7P** 170296-49-8P

170296-50-1P 170296-51-2P 170296-52-3P
 170296-53-4P 170296-54-5P 170296-55-6P 170296-56-7P
 170296-57-8P 170296-58-9P 170296-59-0P 170296-60-3P
 170296-61-4P 170296-62-5P 170296-63-6P 170296-64-7P
 170296-65-8P 170296-66-9P 170296-67-0P 170296-68-1P
 170296-69-2P 170296-70-5P 170296-71-6P 170296-72-7P
 170296-73-8P 170296-74-9P 170296-75-0P 170296-76-1P

170296-77-2P 170296-78-3P 170296-79-4P
 170296-80-7P 170296-81-8P 170296-82-9P
 170296-83-0P 170296-84-1P 170296-85-2P 170296-86-3P
 170296-87-4P 170296-88-5P 170296-89-6P 170296-90-9P
 170296-91-0P 170296-92-1P 170296-93-2P 170296-94-3P
 170296-95-4P 170296-96-5P 170296-97-6P 170296-98-7P
 170296-99-8P 170297-00-4P 170297-01-5P 170297-02-6P
 170297-03-7P 170297-04-8P 170297-05-9P 170297-06-0P
 170297-07-1P 170297-08-2P 170297-09-3P 170297-10-6P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT 95-48-7, reactions 99-89-8, 4-Isopropylphenol 100-51-6, Benzenemethanol, reactions 106-41-2, 4-Bromophenol 106-44-5, reactions 108-39-4, reactions 108-95-2, Phenol, reactions 371-41-5, 4-Fluorophenol 372-20-3, 3-Fluorophenol 459-56-3, 4-Fluorobenzyl alcohol 5441-04-3 57235-35-5, 4,6-Dimethoxypyrimidine-2-thiol 99334-01-7 113583-35-0, 4,6-Dimethoxy-2-methylsulfonylpyrimidine 159559-29-2 159559-91-8
 170297-20-8 170297-29-7 170297-30-0 170297-31-1 170297-32-2
 170297-33-3 170297-34-4 170297-35-5 170297-36-6 170297-37-7
 170297-38-8 170297-39-9 170297-40-2 170297-41-3 170297-42-4
 170297-43-5 170297-44-6

RL: RCT (Reactant)

(carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

IT 159307-92-3P 159307-93-4P 159307-94-5P 159307-95-6P
 159307-96-7P 159307-97-8P 159307-98-9P 159307-99-0P
 159308-00-6P 159308-01-7P 170297-11-7P 170297-12-8P
 170297-13-9P 170297-14-0P 170297-15-1P 170297-16-2P
 170297-17-3P 170297-18-4P 170297-19-5P 170297-21-9P
 170297-22-0P 170297-23-1P 170297-24-2P 170297-25-3P
 170297-26-4P 170297-27-5P 170297-28-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (carboxylic acid derivs. as inhibitors of endothelin binding to receptors)

L8 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 1996 ACS
 AN 1995:234868 HCAPLUS
 DN 122:31550

TI Preparation of 3-(hetero)arylcarboxylic acid-derivative herbicides with increased species selectivity

IN Baumann, Ernst; Rheinheimer, Joachim; Vogelbacher, Uwe Josef; Bratz, Matthias; Theobald, Hans; Gerber, Matthias; Walter, Helmut; Rademacher, Wilhelm; Westphalen, Karl Otto

PA BASF A.-G., Germany

SO Ger. Offen., 25 pp.
CODEN: GWXXBX

PI DE 4313412 A1 941027

AI DE 93-4313412 930423

DT Patent

LA German

IC ICM C07D239-60

ICS C07D401-12; C07C069-66; C07C309-65; C07C309-73; C07D403-12; C07D405-12; C07D409-12; C07D413-12; C07D417-12; C07D491-048; A01N043-54

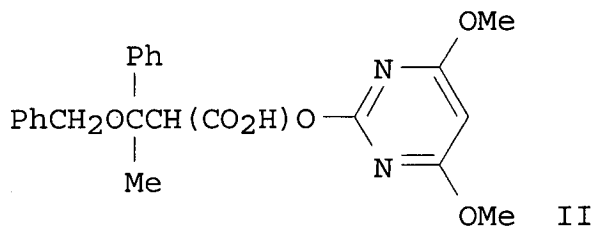
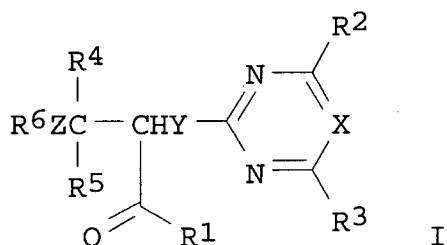
ICA C07D521-00; C07D251-12; C07D307-54; C07D333-24; C07D213-55; C07D277-30; C07D261-08; C07D233-64

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5

OS MARPAT 122:31550

GI

P.D.



AB The title compds. [I; R1 = H, succinylimidoxy, (un)substituted N-contg. 5-member heterocyclic group, etc.; R2, R3 = halogen, C1-4 alkyl or alkoxy or alkylthio, etc.; R4 = (un)substituted Ph, (un)substituted naphthyl, (un)substituted heteroarom. residue, etc.; R5 = H, alkyl, alkenyl, alkynyl, cycloalkyl, Ph, etc.; R6 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl; X = N, (un)substituted CH; Y = direct bond, O, S; Z = O, S], useful as herbicides which have reduced toxicity com. plant species, are prepd. Thus, pyrimidine deriv. II (m.p. 165.degree.; decompn.) was prepd. and demonstrated 10% plant loss when applied to *Gossypium hirsutum* (i.e., cotton) at 0.125 kg/ha, vs. 35% plant loss for a control expt. using I (R1 = OH, R2 = R3 = OMe, R4 = Ph, R5 = R6 = Me, X = CH, Y = Z = O).

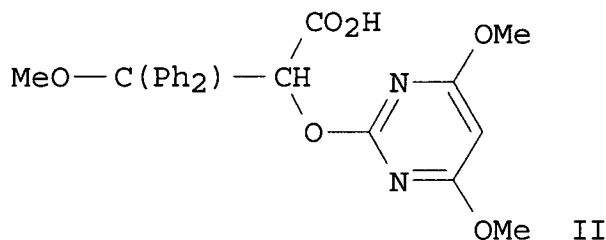
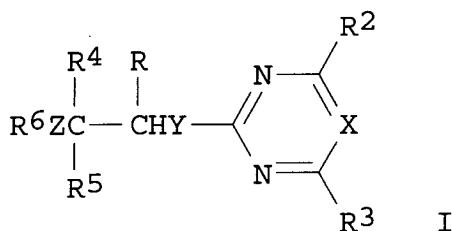
ST selective herbicide prepn pyrimidinylalkylcarboxylic acid;

heteroarylcarboxylic acid deriv herbicide
 IT Herbicides
 (3-(hetero)arylcarboxylic acids)
 IT 159559-10-1P
 RL: AGR (Agricultural use); RCT (Reactant); SPN (Synthetic
 preparation); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (prepn. of 3-(hetero)arylcarboxylic acid-deriv. herbicides with
 increased species selectivity)
 IT 159559-01-0P 159559-02-1P 159559-03-2P 159559-04-3P
 159559-05-4P 159559-06-5P 159559-07-6P 159559-08-7P
 159559-09-8P **159559-11-2P** 159559-12-3P 159559-13-4P
 159559-14-5P 159559-15-6P 159559-16-7P 159559-17-8P
 159559-18-9P 159559-19-0P 159559-20-3P 159559-21-4P
 159559-22-5P 159559-23-6P **159559-24-7P** 159559-25-8P
 159559-26-9P 159559-27-0P 159559-28-1P
 RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL
 (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of 3-(hetero)arylcarboxylic acid-deriv. herbicides with
 increased species selectivity)
 IT 100-51-6, Benzyl alcohol, reactions 5441-04-3 113583-35-0,
 4,6-Dimethoxy-2-methylsulfonylpyrimidine 159559-29-2
 RL: RCT (Reactant)
 (prepn. of 3-(hetero)arylcarboxylic acid-deriv. herbicides with
 increased species selectivity)

=> select rn 18 1-2 hit
 E33 THROUGH E49 ASSIGNED

=> d .ca 19 1-9

L9 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 1996 ACS
 AN 1996:401554 HCAPLUS
 DN 125:58534
 TI Preparation of pyrimidine- and triazine-derivative endothelin
 receptor antagonists
 IN Riechers, Hartmut; Klinge, Dagmar; Amberg, Wilhelm; Kling, Andreas;
 Mueller, Stefan; Baumann, Ernst; Rheinheimer, Joachim; Vogelbacher,
 Uwe Josef; Wernet, Wolfgang; et al.
 PA BASF A.-G., Germany
 SO Ger. Offen., 28 pp.
 CODEN: GWXXBX
 PI DE 19533023 A1 960418
 AI DE 95-19533023 950907
 PRAI DE 94-4436851 941014
 DT Patent
 LA German
 OS MARPAT 125:58534
 GI



AB The title compds. [I; R = CHO, tetrazolyl, CN, CO₂H, groups cleavable to CO₂H; R₂ = (un)substituted NH₂, halogen, (un)substituted alkyl, etc.; R₃ = H, OH, (un)substituted NH₂, halogen, (un)substituted alkyl, etc.; R₄, R₅ = (un)substituted Ph or naphthyl; R₆ = H, alkyl, alkenyl, alkynyl, alkylcarbonyl, (un)substituted Ph, etc.; X = N, (un)substituted CH; Y = direct bond, S, O; Z = S, O, SO, SO₂, direct bond], useful as endothelin receptor antagonists, are prep'd. Thus, pyrimidine deriv. II, m.p. 167.degree., demonstrated a K_i ETA of 6 nM.

IT 178306-68-8P

RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrimidine- and triazine-deriv. endothelin receptor antagonists)

IT 177036-81-6P 177036-86-1P 177036-87-2P
178306-45-1P 178306-46-2P 178306-57-5P
178306-58-6P 178306-59-7P 178306-60-0P
178306-61-1P 178306-64-4P 178306-65-5P
178306-66-6P 178306-67-7P 178306-69-9P
178306-70-2P 178306-71-3P 178306-72-4P
178306-73-5P 178306-74-6P 178306-75-7P
178306-76-8P 178306-77-9P 178306-78-0P
178306-79-1P 178306-80-4P 178306-81-5P
178306-82-6P 178306-83-7P 178306-84-8P
178306-85-9P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrimidine- and triazine-deriv. endothelin receptor antagonists)

IC ICM C07D239-60
ICS C07D239-70; C07D403-12; C07D405-12; C07D491-044; C07D487-04;
C07D495-04; C07D409-12; C07D413-12; C07D417-12; A61K031-41;

A61K031-505

ICA C07D521-00

ICI C07M007-00; C07D491-044, C07D239-00, C07D315-00; C07D487-04,
C07D239-00, C07D209-00

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

IT 178306-68-8P

RL: BAC (Biological activity or effector, except adverse); RCT
(Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL
(Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrimidine- and triazine-deriv. endothelin receptor
antagonists)

IT 177036-81-6P 177036-86-1P 177036-87-2P

177037-02-4P 178306-45-1P 178306-46-2P

178306-57-5P 178306-58-6P 178306-59-7P

178306-60-0P 178306-61-1P 178306-62-2P

178306-63-3P 178306-64-4P 178306-65-5P

178306-66-6P 178306-67-7P 178306-69-9P

178306-70-2P 178306-71-3P 178306-72-4P

178306-73-5P 178306-74-6P 178306-75-7P

178306-76-8P 178306-77-9P 178306-78-0P

178306-79-1P 178306-80-4P 178306-81-5P

178306-82-6P 178306-83-7P 178306-84-8P

178306-85-9P 178306-86-0P 178306-87-1P 178306-88-2P

RL: BAC (Biological activity or effector, except adverse); SPN
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological
study); PREP (Preparation); USES (Uses)

(prepn. of pyrimidine- and triazine-deriv. endothelin receptor
antagonists)

L9 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 1996 ACS

AN 1996:271791 HCAPLUS

DN 125:328

TI Discovery and Optimization of a Novel Class of Orally Active
Nonpeptidic Endothelin-A Receptor Antagonists

AU Riechers, Hartmut; Albrecht, Hans-Peter; Amberg, Willi; Baumann,
Ernst; Bernard, Harald; Boehm, Hans-Joachim; Klinge, Dagmar; Kling,
Andreas; Mueller, Stefan; et al.

CS Hauptlaboratorium, BASF AG, Ludwigshafen, 67056, Germany

SO J. Med. Chem. (1996), 39(11), 2123-8

CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

OS CASREACT 125:328; CJACS-IMAGE; CJACS

AB A novel class of endothelin-A receptor ligands was discovered by
high-throughput screening. Lead structure optimization led to
highly potent antagonists which can be synthesized in a short
sequence. The compds. are endothelin-A-selective, are orally
available, and show a long duration of action.

- IT 171714-84-4P, LU 127043 177036-81-6P
177036-82-7P 177036-83-8P 177036-84-9P
177036-85-0P 177036-86-1P 177036-87-2P
177036-88-3P 177036-89-4P 177036-90-7P
177036-91-8P 177036-93-0P 177036-94-1P
177036-95-2P, LU 134981 177036-96-3P, LU 136181
177036-97-4P 177036-98-5P 177036-99-6P
177037-00-2P
RL: BAC (Biological activity or effector, except adverse); PRP
(Properties); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of a novel class of orally active nonpeptidic
endothelin-a receptor antagonists)
- IT 159308-17-5, LU 110896 170297-04-8, LU 110897
RL: BAC (Biological activity or effector, except adverse); PRP
(Properties); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(prepn. of a novel class of orally active nonpeptidic
endothelin-a receptor antagonists)
- IT 177037-01-3
RL: RCT (Reactant)
(prepn. of a novel class of orally active nonpeptidic
endothelin-a receptor antagonists)
- IT 177036-79-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of a novel class of orally active nonpeptidic
endothelin-a receptor antagonists)
- CC 1-3 (Pharmacology)
Section cross-reference(s): 2, 28
- IT 171714-84-4P, LU 127043 177036-81-6P
177036-82-7P 177036-83-8P 177036-84-9P
177036-85-0P 177036-86-1P 177036-87-2P
177036-88-3P 177036-89-4P 177036-90-7P
177036-91-8P 177036-92-9P 177036-93-0P
177036-94-1P 177036-95-2P, LU 134981
177036-96-3P, LU 136181 177036-97-4P
177036-98-5P 177036-99-6P 177037-00-2P
RL: BAC (Biological activity or effector, except adverse); PRP
(Properties); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of a novel class of orally active nonpeptidic
endothelin-a receptor antagonists)
- IT 159308-17-5, LU 110896 170297-04-8, LU 110897
RL: BAC (Biological activity or effector, except adverse); PRP
(Properties); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(prepn. of a novel class of orally active nonpeptidic
endothelin-a receptor antagonists)
- IT 90-98-2, 4,4'-Dichlorobenzophenone 96-34-4, Chloroacetic acid

methyl ester 119-61-9, Benzophenone, reactions 345-70-0,
 3,3'-Difluorobenzophenone 345-92-6, 4,4'-Difluorobenzophenone
 393-52-2, 2-Fluorobenzoyl chloride 591-17-3, 3-Bromotoluene
 611-97-2, 4,4'-Dimethylbenzophenone 1072-85-1,
 2-Fluorobromobenzene 1711-05-3, 3-Methoxybenzoic acid chloride
 1711-06-4, 3-Methylbenzoyl chloride 2398-37-0,
 3-Methoxybromobenzene 35144-22-0, 2-(Methylsulfonyl)-4,6-
 dimethylpyrimidine 57268-32-3 77166-01-9 113583-35-0,
 2-(Methylsulfonyl)-4,6-dimethoxypyrimidine 143323-12-0
 149228-24-0 **177037-01-3** 177037-02-4 177037-03-5

RL: RCT (Reactant)

(prepn. of a novel class of orally active nonpeptidic
 endothelin-a receptor antagonists)

IT 2852-68-8P, 3,3'-Dimethylbenzophenone 39193-85-6P,
 3,3'-Dimethoxybenzophenone 76527-25-8P 177036-78-1P

177036-79-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of a novel class of orally active nonpeptidic
 endothelin-a receptor antagonists)

L9 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 1996 ACS

AN 1996:237460 HCAPLUS

DN 124:289560

TI Preparation of pyrimidinyl- and triazinyl-oxy and
 thio-3-haloalkyl-propionic acid derivatives as herbicides

IN Luethy, Christoph; Lutz, William

PA Ciba-Geigy A.-G., Switz.

SO PCT Int. Appl., 115 pp.

CODEN: PIXXD2

PI WO 9600219 A1 960104

DS W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG,
 KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU,
 SG, SI, SK, TJ, TM, TT, UA, US, UZ, VN

RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR,
 IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG

AI WO 95-EP2295 950613

PRAI CH 94-2045 940627

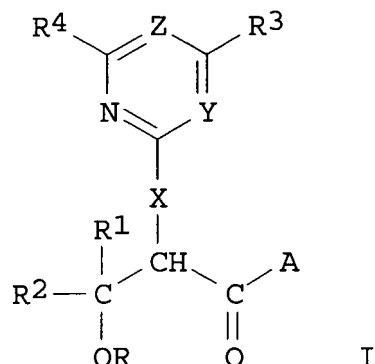
CH 94-2858 940920

DT Patent

LA English

OS MARPAT 124:289560

GI



AB The title compds. [I; A = alkylthio, alkyloxy, OH, (un)substituted heterocyclyl, etc.; R = H, (un)substituted alkyl, haloalkyl, (un)substituted Ph, etc.; R1 = C1-7 haloalkyl; R2 = H, alkyl, alkenyl, cycloalkyl, (un)substituted Ph, pyridyl, thienyl, etc.; R3 = Me, Et, MeO, EtO, CF3O, HCF2O, etc.; R4 = F, Cl, Me, Et, Pr, cyclopropyl, MeO, EtO, etc; X = O, S; Y = N or if Z = N then Y is N, (un)substituted CH; Z = N, (un)substituted CH], useful as selective herbicides esp. for controlling weeds, are prepd. and I-contg. formulations presented. Thus, I (A = OCM₃, R = R2 = Me, R3 = R4 = OMe, X = S, Y = N, Z = CH) was prepd.

IT 175527-71-6P 175527-72-7P

RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrimidinyl- and triazinyl-oxy and thio-3-haloalkyl-propionic acid derivs. as herbicides)

IC ICM C07D239-60

ICS A01N043-40; C07D405-12; C07D401-00; C07D233-54; C07D401-12

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 5

IT	161600-98-2P	164790-07-2P	175527-30-7P	175527-31-8P
	175527-36-3P	175527-37-4P	175527-38-5P	175527-39-6P
	175527-40-9P	175527-41-0P	175527-42-1P	175527-43-2P
	175527-44-3P	175527-45-4P	175527-46-5P	175527-47-6P
	175527-48-7P	175527-49-8P	175527-50-1P	175527-51-2P
	175527-52-3P	175527-53-4P	175527-54-5P	175527-55-6P
	175527-56-7P	175527-57-8P	175527-58-9P	175527-59-0P
	175527-60-3P	175527-61-4P	175527-62-5P	175527-63-6P
	175527-64-7P	175527-65-8P	175527-66-9P	175527-67-0P
	175527-68-1P	175527-69-2P	175527-70-5P	175527-71-6P
	175527-72-7P	175527-73-8P	175527-74-9P	175527-75-0P
	175527-76-1P	175527-77-2P	175527-78-3P	175527-79-4P
	175527-80-7P	175527-81-8P	175527-82-9P	175527-83-0P
	175527-84-1P	175527-85-2P	175527-86-3P	175527-87-4P

Clardy 08/537,843

175527-88-5P	175527-89-6P	175527-90-9P	175527-91-0P
175527-92-1P	175527-93-2P	175527-94-3P	175527-95-4P
175527-96-5P	175527-97-6P	175527-98-7P	175527-99-8P
175528-00-4P	175528-01-5P	175528-02-6P	175528-03-7P
175528-04-8P	175528-05-9P	175528-06-0P	175528-07-1P
175528-08-2P	175528-09-3P	175528-10-6P	175528-11-7P
175528-12-8P	175528-13-9P	175528-14-0P	175528-15-1P
175528-16-2P	175528-17-3P	175528-18-4P	175528-19-5P
175528-20-8P	175528-21-9P	175528-22-0P	175528-23-1P
175528-24-2P	175528-25-3P	175528-26-4P	175528-27-5P
175528-28-6P	175528-29-7P	175528-30-0P	175528-31-1P
175528-32-2P	175528-33-3P	175528-34-4P	175528-35-5P
175528-36-6P	175528-37-7P	175528-38-8P	175528-39-9P
175528-40-2P	175528-41-3P	175528-42-4P	175528-43-5P
175528-44-6P	175528-45-7P	175528-46-8P	175528-47-9P
175528-48-0P	175528-49-1P	175528-50-4P	175528-51-5P
175528-52-6P	175528-53-7P	175528-54-8P	175528-55-9P
175528-56-0P	175528-57-1P	175528-58-2P	175528-59-3P
175528-60-6P	175528-61-7P	175528-62-8P	175528-63-9P
175528-64-0P	175528-65-1P	175528-66-2P	175528-67-3P
175528-68-4P	175528-69-5P	175528-70-8P	175528-71-9P
175528-72-0P	175528-73-1P	175528-74-2P	175528-75-3P
175528-76-4P	175528-77-5P	175528-78-6P	175528-79-7P
175528-80-0P	175528-81-1P	175672-08-9P	175672-09-0P
175672-10-3P	175672-11-4P	175672-12-5P	175672-13-6P
175672-14-7P	175672-15-8P	175672-16-9P	175672-17-0P
175672-18-1P	175672-19-2P		

RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyrimidinyl- and triazinyl-oxy and thio-3-haloalkyl-propionic acid derivs. as herbicides)

L9 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 1996 ACS

AN 1995:966284 HCAPLUS

DN 124:22417

TI Receptor selectivity of endothelin antagonists and prevention of vasoconstriction and endothelin-induced sudden death

AU Raschack, Manfred; Unger, Liliane; Riechers, Hartmut; Klinge, Dagmar

CS Knoll AG, Ludwigshafen, Germany

SO J. Cardiovasc. Pharmacol. (1995), 26(Suppl. 3), S397-S399

CODEN: JCPCDT; ISSN: 0160-2446

DT Journal

LA English

AB The new endothelin (ET) receptor antagonist LU 127043 shows higher ETA affinity than BQ 123, Ro 46 2005, and BMS 182874, with a K_i of 6 nmol/L vs. 19, 28, and 57 nmol/L. ETA/ETB selectivity of LU 127043 of about 160 is comparable to that of BQ 123 (200) and is much greater than that of Ro 46-2005 (0.93) and SB 209670 (0.74). In rabbit aortic segments, LU 127043 showed Et antagonistic potency

similar to that of BQ 123 and BMS 182874 (pA₂ 7.34 vs. 7.36 and 7.09), whereas SB 209670 is more potent (9.80). In rats, LU 127043 completely prevents the ET-1-induced sudden death due to coronary constriction, as indicated by a pronounced T-wave increase. With i.v. pretreatment, LU 127043 is as selective as SB 209670, whereas it is three times more active using 4 h oral pretreatment. Even 8 h after oral administration, LU 127043, in contrast to SB 209670, provides dose-dependent protection. Hence, LU 127043 is an example of a selective ETA antagonist with high oral availability and long duration of action. Because the in vivo efficacy of other high affinity ET antagonists is relatively low, further optimization for therapeutic use should conc. on pharmacokinetic properties.

IT 171714-84-4, LU 127043

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BIOL (Biological study); PROC (Process) (receptor selectivity of endothelin antagonists and prevention of vasoconstriction and endothelin-induced sudden death)

CC 2-10 (Mammalian Hormones)

IT 136553-81-6, BQ 123 150725-87-4, Ro 46-2005 153042-42-3, BMS 182874 157659-79-5, SB 209670 171714-84-4, LU 127043

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BIOL (Biological study); PROC (Process) (receptor selectivity of endothelin antagonists and prevention of vasoconstriction and endothelin-induced sudden death)

L9 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 1996 ACS

AN 1995:667255 HCAPLUS

DN 123:83384

TI Preparation of 3-hydroxycarboxylic acid-derivative herbicides and plant-growth regulators

IN Baumann, Ernst; Rheinheimer, Joachim; Vogelbacher, Uwe Josef; Gerber, Matthias; Rademacher, Wilhelm; Walter, Helmut; Westphalen, Karl-Otto

PA BASF A.-G., Germany

SO Ger. Offen., 26 pp.

CODEN: GWXXBX

PI DE 4335950 A1 950427

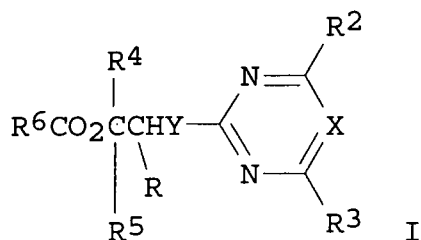
AI DE 93-4335950 931021

DT Patent

LA German

OS MARPAT 123:83384

GI



AB The title compds. [I; R = CHO, CO₂H, CO₂H substituted with a hydrolyzable group; R₂, R₃ = halogen, (un)substituted alkyl, (un)substituted alkoxy, alkylthio; R₄ = (un)substituted alkyl; R₅ = H, alkyl, alkenyl, alkynyl, alkylcarbonyl, cycloalkyl, (un)substituted Ph, etc.; R₆ = (un)substituted alkyl; X = N, (un)substituted CH; Y = O, S] [e.g., Me 3-acetoxy-3-phenyl-2-[(4,6-dimethoxypyrimidin-2-yl)thio]butyrate], useful as herbicides and plant-growth regulators (no data), are prepd.

IT 164790-06-1P

RL: AGR (Agricultural use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 3-hydroxycarboxylic acid-deriv. herbicides and plant-growth regulators)

IT 164790-03-8P

RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 3-hydroxycarboxylic acid-deriv. herbicides and plant-growth regulators)

IC ICM C07D239-46

ICS C07D251-30; C07D401-12; C07D405-12; C07D409-12; C07D411-12; C07D413-12; C07D417-12; A01N043-54; A01N043-66; A01N043-74; A01N043-56

ICI C07D401-12, C07D213-06; C07D251-30; C07D405-12, C07D307-06; C07D239-46; C07D409-12, C07D333-06

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5

IT 164790-06-1P 164790-07-2P

RL: AGR (Agricultural use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 3-hydroxycarboxylic acid-deriv. herbicides and plant-growth regulators)

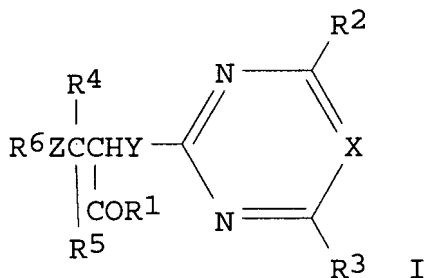
IT 164790-03-8P 164790-04-9P 164790-05-0P 164790-09-4P

RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 3-hydroxycarboxylic acid-deriv. herbicides and

plant-growth regulators)

L9 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 1996 ACS
 AN 1994:700921 HCAPLUS
 DN 121:300921
 TI Preparation of 3-(hetero)aryloxy(thio)carboxylic acid derivatives as agrochemical herbicides
 IN Baumann, Ernst; Rheinheimer, Joachim; Vogelbacher, Uwe Josef; Bratz, Matthias; Meyer, Norbert; Gerber, Matthias; Walter, Helmut; Rademacher, Wilhelm; Westphalen, Karl Otto
 PA BASF A.-G., Germany
 SO Ger. Offen., 26 pp.
 CODEN: GWXXBX
 PI DE 4313416 A1 941027
 AI DE 93-4313413 930423
 DT Patent
 LA German
 OS MARPAT 121:300921
 GI



AB The title compds. [I; R1 = H, succinimidyloxy residue, (un)substituted N-contg. 5-membered heterocyclic residue, etc.; R2, R3 = halogen, alkyl, alkoxy, thioalkyl, etc.; R4 = C1-10 alkyl contg. 1-5 halogen atom(s), (un)substituted heterocyclyl residue, (un)substituted Ph or naphthyl, etc.; R5 = H, alkyl, alkenyl, alkynyl, cycloalkyl, etc.; R6 = (un)substituted Ph or naphthyl, (un)substituted heteroaryl, etc.; X = undefined (sic); Y = direct bond, O, S; Z = S, O] (e.g., R1-R3 = OMe, R4 = R6 = Ph, R5 = Me, X = CH, Y = Z = O; m.p. 100-103.degree.), useful as agrochem. herbicides for the control of unwanted plants in crop fields, are prepd. and a I-contg. formulation presented.

IT 159308-02-8P

RL: AGR (Agricultural use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 3-(hetero)aryloxy(thio)carboxylic acid derivs. as

agrochem. herbicides)

IT 159308-03-9P 159308-04-0P 159308-05-1P
 159308-06-2P 159308-07-3P 159308-08-4P
 159308-09-5P 159308-10-8P 159308-11-9P
 159308-12-0P 159308-13-1P 159308-14-2P
 159308-15-3P 159308-16-4P 159308-17-5P
 159308-18-6P 159308-19-7P
 RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL
 (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of 3-(hetero)aryloxy(thio)carboxylic acid derivs. as
 agrochem. herbicides)

IC ICM C07D239-60
 ICS C07D251-26; C07D405-12; C07D409-12; C07D491-048; C07D403-12;
 C07D417-12; C07D413-12; C07D413-14; C07D401-12; A01N043-54;
 A01N043-66

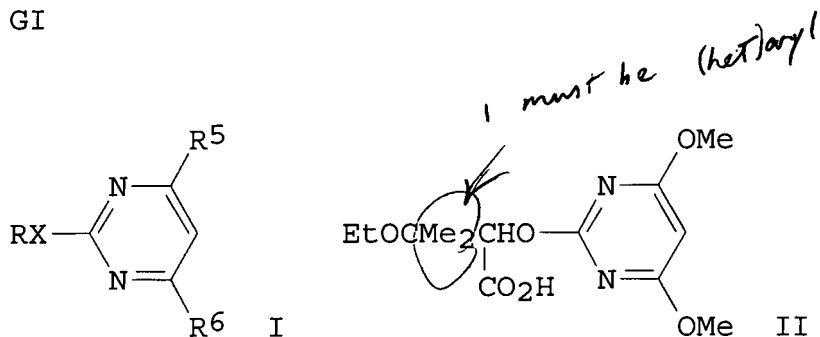
ICA C07D521-00; C07D333-24; C07D307-54
 ICI C07D405-12, C07D239-60, C07D251-26, C07D307-54; C07D409-12
 CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 5

IT 159308-02-8P
 RL: AGR (Agricultural use); RCT (Reactant); SPN (Synthetic
 preparation); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (prepn. of 3-(hetero)aryloxy(thio)carboxylic acid derivs. as
 agrochem. herbicides)

IT 159308-03-9P 159308-04-0P 159308-05-1P
 159308-06-2P 159308-07-3P 159308-08-4P
 159308-09-5P 159308-10-8P 159308-11-9P
 159308-12-0P 159308-13-1P 159308-14-2P
 159308-15-3P 159308-16-4P 159308-17-5P
 159308-18-6P 159308-19-7P
 RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL
 (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of 3-(hetero)aryloxy(thio)carboxylic acid derivs. as
 agrochem. herbicides)

L9 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 1996 ACS
 AN 1992:448600 HCAPLUS
 DN 117:48600
 TI Preparation of 3-alkoxy-2-pyrimidyloxy- and -thioalkanoates as
 herbicides
 IN Harada, Katsumasa; Abe, Takaaki; Akiyoshi, Yuji; Shiraishi, Hiroshi;
 Yamamoto, Kaoru
 PA Ube Industries, Ltd., Japan
 SO Eur. Pat. Appl., 65 pp.
 CODEN: EPXXDW
 PI EP 481512 A1 920422
 DS R: DE, FR, GB, IT
 AI EP 91-117829 911018

PRAI JP 90-279328 901019
 JP 91-189613 910423
 DT Patent
 LA English
 OS MARPAT 117:48600
 GI



AB Title compds. [I; R = R1OCR2R3CH(CO2R4); R1 = (cyclo)alkyl, alkenyl, alkynyl, haloalkyl, cyanoalkyl; R2 = H, alkyl; R3 = (cyclo)alkyl; R2R3 = atoms to complete a carbocyclic ring; R4 = H, alkyl, alkynyl; R5 = (halo)alkyl, alkoxy, halo; R6 = alkyl, alkoxy; X = O, S] were prepd. Thus, Et 2,3-epoxy-3-methylbutanoate was treated with H2SO4 in EtOH and the product condensed with 4,6-dimethoxy-2-methylsulfonylpyrimidine to give, after sapon., title compd. II which gave complete control of 5 weeds, e.g., crabgrass, with slight damage to cotton at 20 g/are preemergent.

IT 142411-65-2P 142411-66-3P 142411-99-2P
 142412-00-8P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of, as herbicide)

IC ICM C07D239-60

ICS C07D239-52; C07D239-34; A01N043-54

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 5

IT	134433-11-7P	134433-27-5P	142411-45-8P	142411-46-9P
	142411-47-0P	142411-48-1P	142411-49-2P	142411-50-5P
	142411-51-6P	142411-52-7P	142411-53-8P	142411-54-9P
	142411-55-0P	142411-56-1P	142411-57-2P	142411-58-3P
	142411-59-4P	142411-60-7P	142411-61-8P	142411-62-9P
	142411-63-0P	142411-64-1P	142411-65-2P	
	142411-66-3P	142411-67-4P	142411-68-5P	142411-69-6P
	142411-70-9P	142411-71-0P	142411-72-1P	142411-73-2P
	142411-74-3P	142411-75-4P	142411-76-5P	142411-77-6P
	142411-78-7P	142411-79-8P	142411-80-1P	142411-81-2P
	142411-82-3P	142411-83-4P	142411-84-5P	142411-85-6P
	142411-86-7P	142411-87-8P	142411-88-9P	142411-89-0P

Clardy 08/537,843

142411-90-3P	142411-91-4P	142411-92-5P	142411-93-6P
142411-94-7P	142411-95-8P	142411-96-9P	142411-97-0P
142411-98-1P	142411-99-2P	142412-00-8P	
142412-01-9P	142412-02-0P	142412-03-1P	142412-04-2P
142412-05-3P	142412-06-4P	142412-07-5P	142412-08-6P
142412-09-7P	142412-10-0P	142412-11-1P	142412-12-2P
142412-13-3P	142412-14-4P	142412-15-5P	142412-16-6P
142412-17-7P	142412-18-8P	142412-19-9P	142412-20-2P
142412-21-3P	142412-22-4P	142412-23-5P	142412-24-6P
142412-25-7P	142412-26-8P	142412-27-9P	142412-28-0P
142412-29-1P	142412-30-4P	142412-31-5P	142412-32-6P
142412-33-7P	142412-34-8P	142412-35-9P	142412-36-0P
142412-37-1P	142412-38-2P	142412-39-3P	142412-40-6P
142412-41-7P	142412-42-8P	142412-43-9P	142412-44-0P
142412-45-1P	142412-46-2P	142412-47-3P	142412-48-4P
142412-49-5P	142412-50-8P	142412-51-9P	142412-52-0P
142412-53-1P	142412-54-2P	142412-55-3P	142412-56-4P
142412-57-5P	142412-58-6P	142412-59-7P	142412-60-0P
142412-61-1P	142412-62-2P	142412-63-3P	142412-64-4P
142412-65-5P	142412-66-6P	142412-67-7P	142412-68-8P
142412-69-9P	142412-70-2P	142412-71-3P	142412-72-4P
142412-73-5P	142412-74-6P	142412-75-7P	142412-76-8P
142412-77-9P	142412-78-0P	142412-79-1P	142412-80-4P
142412-81-5P	142412-82-6P	142412-83-7P	142412-84-8P
142412-85-9P	142412-86-0P	142412-87-1P	142412-88-2P
142412-89-3P	142412-90-6P	142412-91-7P	142412-92-8P
142412-93-9P	142412-94-0P	142412-95-1P	142412-96-2P
142412-97-3P	142412-98-4P	142412-99-5P	142413-00-1P
142413-01-2P	142413-02-3P	142413-03-4P	142413-04-5P
142413-05-6P	142413-06-7P	142413-07-8P	142430-08-8P
142430-09-9P	142430-10-2P	142430-11-3P	142430-12-4P
142430-13-5P			

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as herbicide)

L9 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 1996 ACS

AN 1991:429369 HCAPLUS

DN 115:29369

TI Preparation of 2-aryl-2-(2-pyrimidinylloxy)acetates and analogs as agrochemicals

IN Wegner, Peter; Harde, Christoph; Nordhoff, Erhard; Krueger, Anita; Krueger, Gabriele; Tarara, Gerhard; Heinrich, Nikolaus; Rees, Richard; Johann, Gerhard; Koetter, Clemens

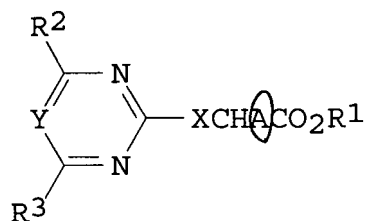
PA Schering A.-G., Fed. Rep. Ger.

SO Eur. Pat. Appl., 26 pp.

CODEN: EPXXDW

PI EP 409368 A2 910123

DS R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE
 AI EP 90-250184 900719
 PRAI DE 89-3924259 890719
 DE 90-4009481 900322
 DT Patent
 LA German
 OS MARPAT 115:29369
 GI



AB The title compds. [I; A = (halo)alkyl, alkenyl, cycloalkyl, PhCH₂, (un)substituted Ph, pyridyl, naphthyl, etc.; R₁ = H, alkyl, PhCH₂; R₂, R₃ = alkyl, alkoxy, alkylthio, (di)alkylamino, halo; X = O, S; Y = CH, N] were prepd. as agrochem. fungicides, herbicides, and plant growth regulators. Thus, MeSO₂OR (R = 4,6-dimethoxypyrimidinyl) was condensed with HSCH₂CO₂Me and the product condensed with CH₂:CHCH₂Br to give CH₂:CHCH₂CH(OR)CO₂Me. ROCHPhCO₂Me gave 75-89% control of 5 weeds (e.g. Abutilon theophrasti) at 1.0 kg/ha postemergent.

IT **134433-24-2P 134461-60-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as agrochem.)

IC ICM C07D239-60

ICS C07D401-12; C07D251-30; C07D251-38; C07D403-12; C07D405-12;
 C07D409-12; C07D251-46; A01N043-54; A01N043-66

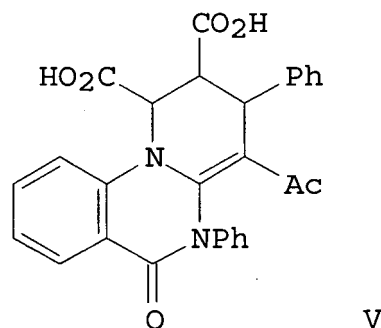
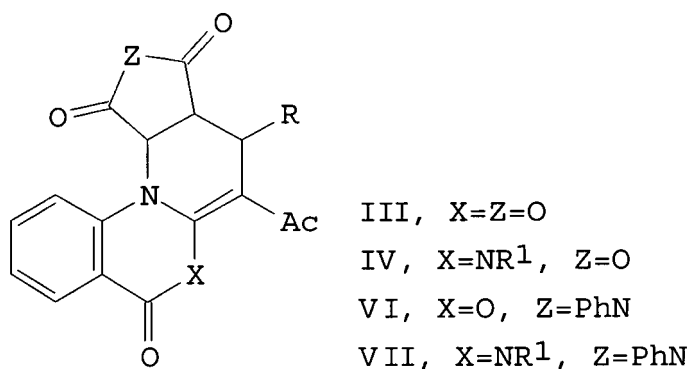
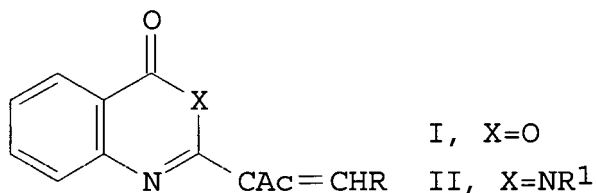
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 5

IT	127091-57-0P	127091-63-8P	127091-73-0P	127091-77-4P
	127091-78-5P	133458-29-4P	133458-30-7P	133458-32-9P
	133458-34-1P	133483-96-2P	133483-97-3P	134432-62-5P
	134432-63-6P	134432-64-7P	134432-65-8P	134432-66-9P
	134432-67-0P	134432-68-1P	134432-69-2P	134432-70-5P
	134432-71-6P	134432-72-7P	134432-73-8P	134432-74-9P
	134432-75-0P	134432-76-1P	134432-77-2P	134432-78-3P
	134432-79-4P	134432-80-7P	134432-81-8P	134432-82-9P
	134432-83-0P	134432-84-1P	134432-85-2P	134432-86-3P
	134432-87-4P	134432-88-5P	134432-89-6P	134432-90-9P
	134432-91-0P	134432-92-1P	134432-93-2P	134432-94-3P
	134432-95-4P	134432-96-5P	134432-97-6P	134432-98-7P
	134432-99-8P	134433-00-4P	134433-01-5P	134433-02-6P

134433-03-7P 134433-04-8P 134433-05-9P 134433-06-0P
 134433-07-1P 134433-08-2P 134433-09-3P 134433-10-6P
 134433-11-7P 134433-12-8P 134433-13-9P 134433-14-0P
 134433-15-1P 134433-16-2P 134433-17-3P 134433-18-4P
 134433-19-5P 134433-20-8P 134433-21-9P 134433-22-0P
 134433-23-1P **134433-24-2P** 134433-25-3P 134433-26-4P
 134433-27-5P 134433-28-6P 134461-59-9P **134461-60-2P**
 134461-61-3P 134461-62-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as agrochem.)

L9 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 1996 ACS
 AN 1981:515443 HCAPLUS
 DN 95:115443
 TI Synthesis and reactions of 2-(.alpha.-acetylstyryl)-3,1-benzoxazin-
 (4H)-ones and 2-(.alpha.-acetylstyryl)-quinazolin-4-(3H)-ones
 AU Elkasaby, M. A.; Nouredin, N. A.
 CS Fac. Sci., Ain Shams Univ., Cairo, Egypt
 SO Indian J. Chem., Sect. B (1981), 20B(4), 290-3
 CODEN: IJSBDB; ISSN: 0376-4699
 DT Journal
 LA English
 GI



AB Benzoxazinones I (R = Ph, p-MeOC₆H₄, p-Me₂NC₆H₄) and quinazolines II (R = Ph, p-MeOC₆H₄; R₁ = H, Ph, p-MeC₆H₄, p-MeOC₆H₄) were prepd. from o-HO₂CC₆H₄NHCOAc:CHR. I (R = Ph, p-MeOC₆H₄) react with maleic anhydride to give furopyridobenzoxazines III. Several II similarly underwent Diels-Alder reaction with maleic anhydride to give the furopyridoquinazolines IV. IV (R = R₁ = Ph) was hydrolyzed to give the pyridoquinazoline V. II and III reacted with N-phenylmaleimide to give cycloadducts VI and VII, resp. Reaction of I with Grignard reagent and II with PhSH were investigated.

IT 78817-76-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 70723-69-2P 78817-52-4P 78817-55-7P 78817-56-8P 78817-57-9P
78817-58-0P 78817-60-4P 78817-61-5P 78817-62-6P 78817-63-7P
78817-64-8P 78817-65-9P 78817-66-0P 78817-67-1P 78817-68-2P
78817-69-3P 78817-70-6P 78817-71-7P 78817-72-8P 78817-73-9P
78817-74-0P 78817-75-1P 78817-76-2P 78817-77-3P
78817-78-4P 78817-79-5P 78834-04-5P 78852-97-8P 78922-69-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

=> fil reg

FILE "REGISTRY" ENTERED AT 07:43:57 ON 05 SEP 96
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 1996 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 02 SEPT 96 HIGHEST RN 180310-23-0
DICTIONARY FILE UPDATES: 04 SEPT 96 HIGHEST RN 180310-23-0

TSCA INFORMATION NOW CURRENT THROUGH DECEMBER 1995

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

=> s-e33-49

1 159559-11-2/BI
(159559-11-2/RN)
1 159559-24-7/BI
(159559-24-7/RN)
1 170296-16-9/BI
(170296-16-9/RN)
1 170296-36-3/BI
(170296-36-3/RN)
1 170296-42-1/BI
(170296-42-1/RN)
1 170296-44-3/BI
(170296-44-3/RN)
1 170296-46-5/BI

Clardy 08/537,843

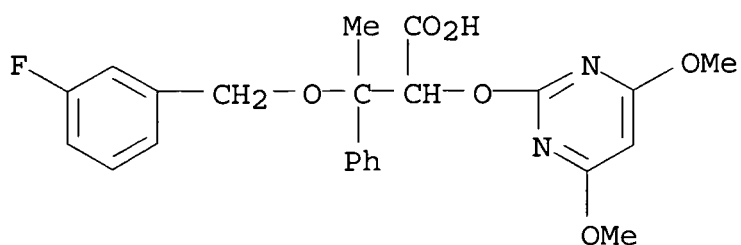
```
(170296-46-5/RN)
1 170296-48-7/BI
  (170296-48-7/RN)
1 170296-50-1/BI
  (170296-50-1/RN)
1 170296-52-3/BI
  (170296-52-3/RN)
1 170296-54-5/BI
  (170296-54-5/RN)
1 170296-60-3/BI
  (170296-60-3/RN)
1 170296-72-7/BI
  (170296-72-7/RN)
1 170296-77-2/BI
  (170296-77-2/RN)
1 170296-79-4/BI
  (170296-79-4/RN)
1 170296-81-8/BI
  (170296-81-8/RN)
1 170296-82-9/BI
  (170296-82-9/RN)
L10      17 (159559-11-2/BI OR 159559-24-7/BI OR 170296-16-9/BI OR 170
          296-36-3/BI OR 170296-42-1/BI OR 170296-44-3/BI OR 170296-
          46-5/BI OR 170296-48-7/BI OR 170296-50-1/BI OR 170296-52-3
          /BI OR 170296-54-5/BI OR 170296-60-3/BI OR 170296-72-7/BI
          OR 170296-77-2/BI OR 170296-79-4/BI OR 170296-81-8/BI OR 1
          70296-82-9/BI)
```

```
=> d id ecan 1-17
'ID' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'ECAN' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
ENTER DISPLAY FORMAT (IDE):end
```

```
=> d ide can l10 1-17
```

```
L10  ANSWER 1 OF 17  REGISTRY  COPYRIGHT 1996 ACS
RN    170296-82-9  REGISTRY
CN    Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-
      .beta.-[(3-fluorophenyl)methoxy]-.beta.-methyl-, sodium salt (9CI)
      (CA INDEX NAME)
MF    C23 H23 F N2 O6 . Na
SR    CA
LC    STN Files:   CA, CAPLUS, TOXLIT
CRN   (170296-81-8)
```

Clardy 08/537,843



● Na

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 2 OF 17 REGISTRY COPYRIGHT 1996 ACS

RN 170296-81-8 REGISTRY

CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-
.beta.-[(3-fluorophenyl)methoxy]-.beta.-methyl- (9CI) (CA INDEX
NAME)

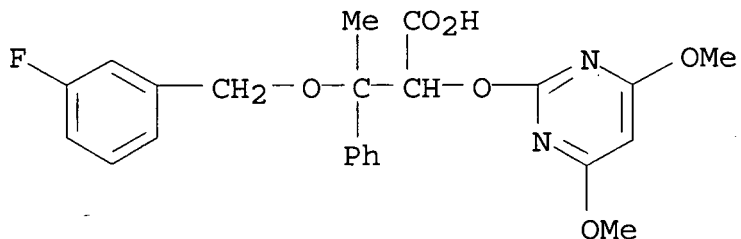
FS 3D CONCORD

MF C23 H23 F N2 O6

CI COM

SR CA

LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

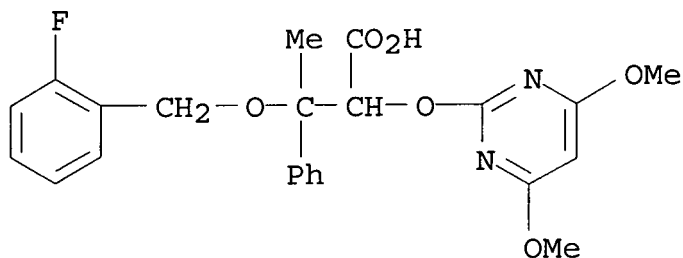
REFERENCE 1: 123:307319

L10 ANSWER 3 OF 17 REGISTRY COPYRIGHT 1996 ACS

RN 170296-79-4 REGISTRY

Clardy 08/537,843

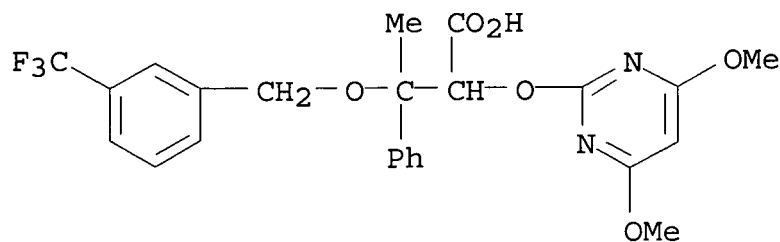
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy] -
.beta.-[(2-fluorophenyl)methoxy] - .beta.-methyl- (9CI) (CA INDEX
NAME)
FS 3D CONCORD
MF C23 H23 F N2 O6
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

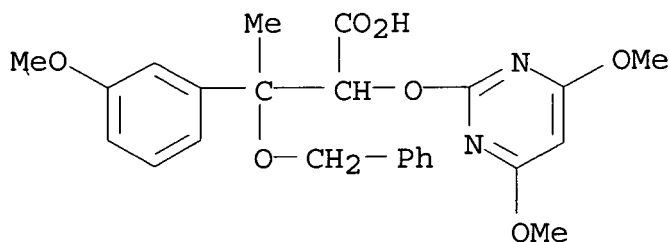
L10 ANSWER 4 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN 170296-77-2 REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy] -
.beta.-methyl- .beta.-[[3-(trifluoromethyl)phenyl]methoxy] - (9CI)
(CA INDEX NAME)
FS 3D CONCORD
MF C24 H23 F3 N2 O6
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

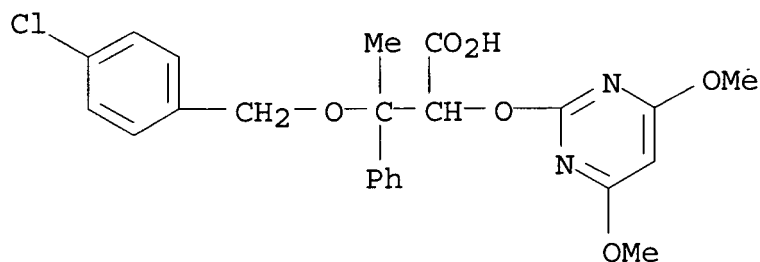
L10 ANSWER 5 OF 17 REGISTRY COPYRIGHT 1996 ACS
 RN 170296-72-7 REGISTRY
 CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-3-methoxy-.beta.-methyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C24 H26 N2 O7
 SR CA
 LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 6 OF 17 REGISTRY COPYRIGHT 1996 ACS
 RN 170296-60-3 REGISTRY
 CN Benzenepropanoic acid, .beta.-[(4-chlorophenyl)methoxy]-.alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.-methyl- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C23 H23 Cl N2 O6
 SR CA
 LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 7 OF 17 REGISTRY COPYRIGHT 1996 ACS

RN 170296-54-5 REGISTRY

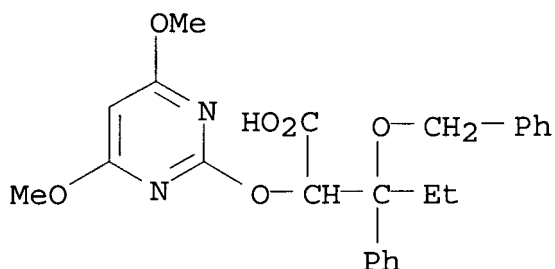
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-
.beta.-ethyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C24 H26 N2 O6

SR CA

LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 8 OF 17 REGISTRY COPYRIGHT 1996 ACS

RN 170296-52-3 REGISTRY

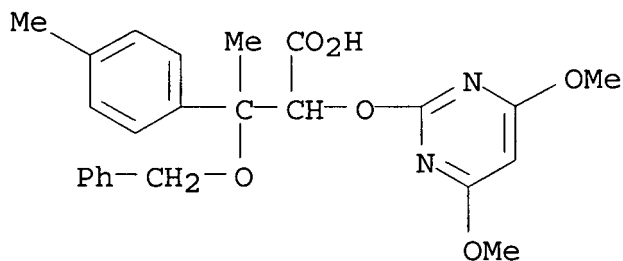
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-
.beta.,4-dimethyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C24 H26 N2 O6

SR CA

LC STN Files: CA, CAPLUS, TOXLIT

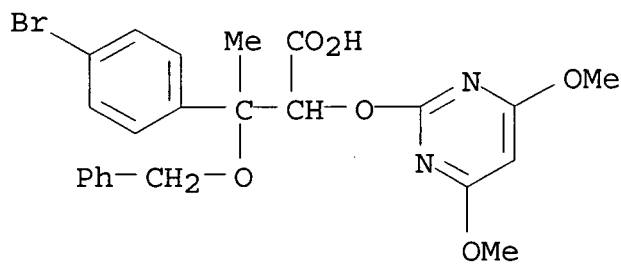


Clardy 08/537,843

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 9 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN 170296-50-1 REGISTRY
CN Benzenepropanoic acid, 4-bromo-.alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.-methyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H23 Br N2 O6
SR CA
LC STN Files: CA, CAPLUS, TOXLIT

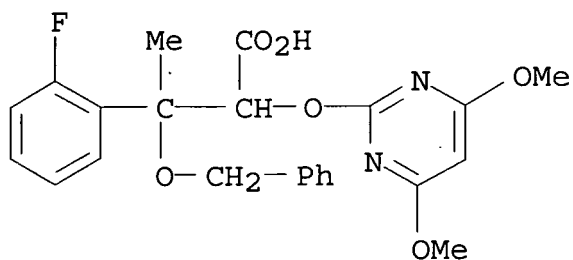


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 10 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN 170296-48-7 REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-2-fluoro-.beta.-methyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H23 F N2 O6
SR CA
LC STN Files: CA, CAPLUS, TOXLIT

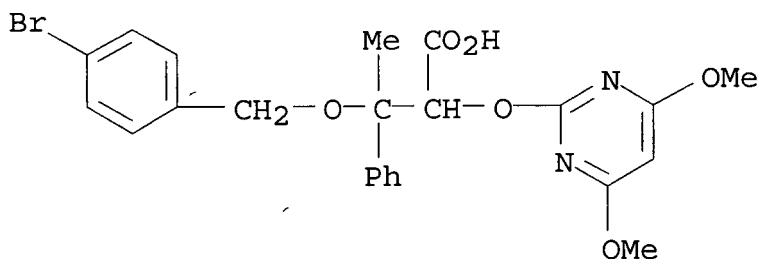
Clardy 08/537,843



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 11 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-46-5** REGISTRY
CN Benzenepropanoic acid, .beta.-[(4-bromophenyl)methoxy]-.alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H23 Br N2 O6
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



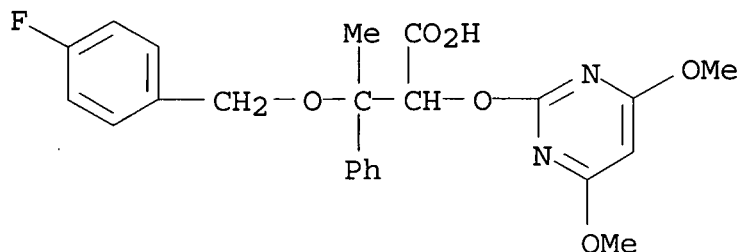
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 12 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-44-3** REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.-[(4-fluorophenyl)methoxy]-.beta.-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H23 F N2 O6
SR CA

Clardy 08/537,843

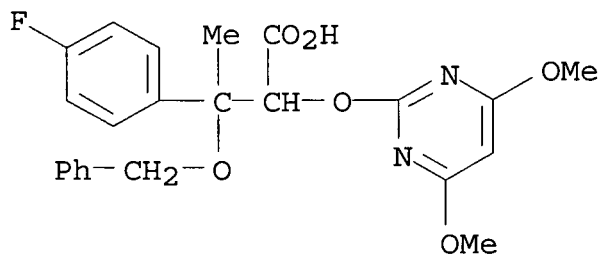
LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 13 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-42-1** REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-4-fluoro-.beta.-methyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H23 F N2 O6
SR CA
LC STN Files: CA, CAPLUS, TOXLIT



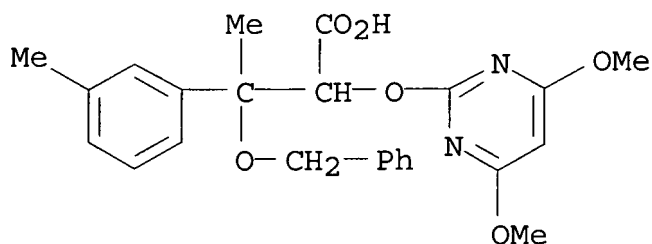
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 14 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN **170296-36-3** REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-.beta.,3-dimethyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H26 N2 O6

Clardy 08/537,843

SR CA
LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 15 OF 17 REGISTRY COPYRIGHT 1996 ACS

RN 170296-16-9 REGISTRY

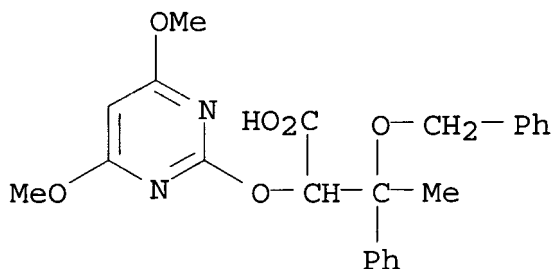
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-
.beta.-methyl-.beta.-(phenylmethoxy)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C23 H24 N2 O6

SR CA

LC STN Files: CA, CAPLUS, TOXLIT



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:307319

L10 ANSWER 16 OF 17 REGISTRY COPYRIGHT 1996 ACS

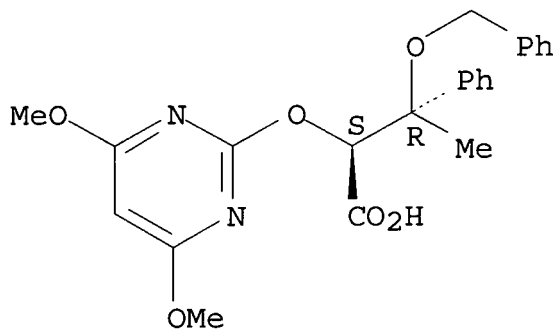
RN 159559-24-7 REGISTRY

CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-
.beta.-methyl-.beta.-(phenylmethoxy)-, (R*,S*)- (9CI) (CA INDEX

Clardy 08/537,843

NAME)
FS STEREOSEARCH
MF C23 H24 N2 O6
SR CA
LC STN Files: CA, CAPLUS
DES 2:R*,S*

Relative stereochemistry.



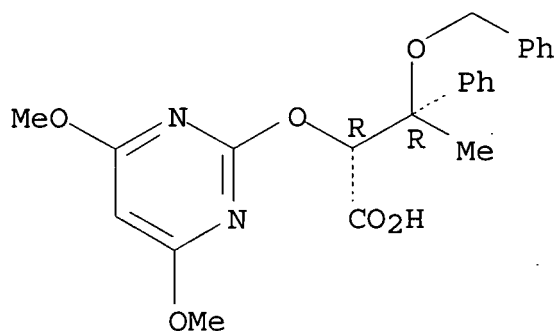
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:31550

L10 ANSWER 17 OF 17 REGISTRY COPYRIGHT 1996 ACS
RN 159559-11-2 REGISTRY
CN Benzenepropanoic acid, .alpha.-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-
.beta.-methyl-.beta.-(phenylmethoxy)-, (R*,R*)- (9CI) (CA INDEX
NAME)
FS STEREOSEARCH
MF C23 H24 N2 O6
SR CA
LC STN Files: CA, CAPLUS
DES 2:R*,R*

Relative stereochemistry.

Clardy 08/537,843



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:31550

=> fil caold

FILE 'CAOLD' ENTERED AT 07:44:24 ON 05 SEP 96
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 1996 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1957-1966

FILE LAST UPDATED: 30 OCT 91 (910803/ED)

To help control your online searching costs, consider using the
HCAOLD File when conducting SmartSELECT searches with large
numbers of terms.

=> d que l11

L2 190 SEA FILE=REGISTRY SSS FUL L1
L11 0 SEA FILE=CAOLD L2